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MOLECULAR DYNAMIC SHOCK WAVE STUDIES IN SOLIDS - FRACTURE AND C-ETC(U)

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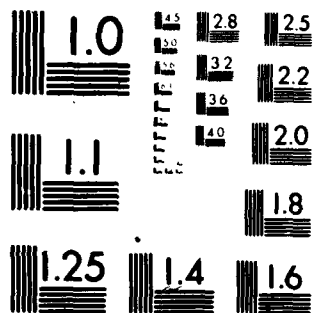
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Fracture and Crack Propagation Shock Waves in Solids			
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)			
The earlier computer simulations of shock waves in solids was completed. An equation of state for shock waves in solids was developed and found to be an accurate description of shock wave properties. Computer simulation techniques were also used to study fracture and crack propagation in solids. The basic assumptions made in the usual continuum mechanics calculations were examined and found to be at best approximate. Some interesting results were found for rapidly applied stresses.			

Final Report - Computer Simulation of Shock Waves in Solids

The early portion of the research effort was devoted to using computer simulation techniques to study shock waves in solids. It was first demonstrated that the computer simulation techniques gave meaningful results by comparison with theory and experiment. The simulations were then used to provide information that could be used to test an equation of state. The research effort was successful on all counts. We shall list here the important contributions that resulted from these studies.

1. The Hugoniot conservation equations are basic to studying shock waves. Originally formulated for fluids, we showed how by appropriate averaging techniques, including the anisotropic properties of solids, they should be modified for solids.

2. An equation of state was formulated using a self-consistent cell approach. This provided an accurate description of the properties of solids at high compression and high temperatures. Comparison with data shows that this provides the best theoretical equation of state today.

3. Computer simulations were used to study the shock wave front. It was found to have interesting structural and potential-dependent properties.

As a result of these computer simulations studies, we now believe that we understand to a high degree of accuracy what is occurring at regions far behind the shock front where equilibrium conditions exist. The region near the shock front is still not understood in solids and should be a future direction for research.

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Fracture and Crack Propagation

The major research effort supported by the grant has been directed towards understanding brittle fracture from an atomistic point of view.

In recent years there has been some effort directed towards lattice statics calculations of fracture. While this is certainly an advance over the continuum approach, there are still many problems of fracture that cannot be answered by the lattice statics approach. Several researchers have recently extended atomistic calculations to treat the dynamic aspects of fracture. Our work follows and extends the earlier Sanders, Weiner and Pear and Ashurst and Hoover dynamic simulations of fracture. The major advance in our work is to use a more realistic potential on a larger sample with no boundary constraints. Thus, we expected to be able to study dislocation formation during crack propagation, as well as other quantitative features of fracture and crack propagation. From this point of view the effort was quite fruitful. We were able to observe dislocation formation during fracture and correlate this feature of fracture with quantitative calculations of brittle vs ductile behavior. We were also able to test some of the most fundamental equations for fracture and found that they were not universally true and at best only approximate. To quote from an article reporting some of these results in the Physical Review Letters April 7, 1980,

"Computer simulations of crack properties were performed on a two-dimensional triangular lattice with a Lennard-Jones interatomic interaction. The use of a long-range potential and an unconstrained sample revealed novel features compared to earlier simulations. The Griffith energy treatment for fracture was found wanting. This system is brittle at low stresses in agreement with the Rice-Thomson criterion and shows dislocation formation at elevated stresses."

While this preliminary report has been published an extensive paper is being written which gives all the details and results of the calculations. This work was the basis for a Ph.D. thesis of one student and an extension of this work will provide a thesis for another student.

computer simulations were also used to study the equation of state for s over a wide range of temperatures and a wide range of compressions. oretical model for the equation of state for solids has been developed. s proved successful in describing both our computer results and experi- l data for such materials as iron and copper. Its particular value is e high pressure and high temperature regime where our equation of state to be better than more complicated first principle calculations. It ing extended to compounds and alloys, where such a fundamental equation ate has not hitherto been available.